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09/502,133	02/11/2000	Harold E. Helson	103544.127	4787
<div>7590      08/09/2007</div> <div>Jason A. Reyes Hale and Dorr LLP 60 State Street Boston, MA 02109</div> <div>EXAMINER JONES, HUGH M</div> <div>ART UNIT      PAPER NUMBER</div> <div>2128</div> <div>MAIL DATE      DELIVERY MODE</div> <div>08/09/2007      PAPER</div>				

**Please find below and/or attached an Office communication concerning this application or proceeding.**

The time period for reply, if any, is set in the attached communication.

<b>Office Action Summary</b>	<b>Application No.</b> 09/502,133	<b>Applicant(s)</b> HELSON	
	<b>Examiner</b> Hugh Jones	<b>Art Unit</b> 2128	

**-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --**

### Period for Reply

**A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.**

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

### Status

- 1) ☒ Responsive to communication(s) filed on 23 May 2007.
- 2a) ☒ This action is **FINAL**.                      2b) ☐ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

### Disposition of Claims

- 4) ☒ Claim(s) 1,5,9 and 13-27 is/are pending in the application.
- 4a) Of the above claim(s) \_\_\_\_\_ is/are withdrawn from consideration.
- 5) ☐ Claim(s) \_\_\_\_\_ is/are allowed.
- 6) ☒ Claim(s) 1,5,9 and 13-27 is/are rejected.
- 7) ☐ Claim(s) \_\_\_\_\_ is/are objected to.
- 8) ☐ Claim(s) \_\_\_\_\_ are subject to restriction and/or election requirement.

### Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☒ The drawing(s) filed on 11 February 2000 is/are: a) ☒ accepted or b) ☐ objected to by the Examiner.  
     Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  
     Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

### Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All    b) ☐ Some \*    c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
2. ☐ Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.
3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

\* See the attached detailed Office action for a list of the certified copies not received.

### Attachment(s)

- |  |   |
|--|---|
| 1) <input type="checkbox"/> Notice of References Cited (PTO-892)   | 4) <input type="checkbox"/> Interview Summary (PTO-413)<br>Paper No(s)/Mail Date. _____ |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948)   | 5) <input type="checkbox"/> Notice of Informal Patent Application                       |
| 3) <input checked="" type="checkbox"/> Information Disclosure Statement(s) (PTO/SB/08)<br>Paper No(s)/Mail Date <u>5/23/2007</u> . | 6) <input type="checkbox"/> Other: _____  |

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**DETAILED ACTION**

1. Claims 1, 5, 9, 13-27 of U. S. Patent 09/502,133 are in front of the office for consideration and remain pending.

**Claim Rejections - 35 USC § 102**

2. The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(b) the invention was patented or described in a printed publication in this or a foreign country or in public use or on sale in this country, more than one year prior to the date of application for patent in the United States.

3. Claims 1, 5, 9, 13-27 are rejected under 35 U.S.C. 102(b) as being clearly anticipated by Helson (The inventor's PhD thesis - of record).
4. The table of contents disclose:

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5. Helson discloses:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure

(fig. 4.5; chapter 4; fig. 3.5, pg. 221, fig. 4.9, fig. 5.4);

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds (page 246; fig. 4.5; chapter 4, fig. 4.9, 5.4);

positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry (page 246; fig. 4.5; chapter 3).

As for dependent claims, see pp. 169, 155-156, 173-212 (redrawing), 207-209, 227-230 (redrawing), table 4.3 (example of candidates); chapter 3 (redrawing) chapter 4 (examples of symmetry).

6. Also see:

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ISI	sym	Identification of Identical Structures
IVP	sym	Iterative Vertex Partitioning
MA	sym	Morgan algorithm
RSCT	SDG	Ring Symmetry Conversion Table
SDCO	sym	Symmetry-derived canonical order
SDG	SDG	Structure Diagram Generation ( <i>q.v.</i> )
SP	sym	Symmetry Perception
SRAB	sym	Symmetry-Reduced A/B

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**Connection Table** The different connection tables used by CAMEO are:

- a) CSS. The ordinary structure storage format. Consists of a list of atoms, with coordinates, element type and charge, and bonds, with the atom pair forming the bond, order, and stereochemistry.
- b) CNAB. During translation of a chemical name (see Graphics chpt.) a simplified, compact CT is built up. Its principal omission is atom coordinates.
- c) Morgan Table. The Morgan table is a data structure similar to that used in the MA. It is used during the search for the canonical table.
- d) Canonical Connection Table (CCT). A highly encoded data structure similar to the Morgan Table in which the structures' A/B's have been canonically sequenced. It is possible to tell if two structures are identical or not by comparing their CCT's.

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**Perception** The process in which the A/B of a structure is examined to deduce higher level information, such as the presence and location of different element types (oxygen, silicon, etc.), rings, aromaticity, stereochemistry, symmetry, and the *canonical connection table*.

**Perception-Derived Structure** See *Derived Structure*

**Perception Phase** (Graphics) There are five distinct occasions when perception is performed: 1) sketch-time; 2) other graphics-time; 3) pre-mechanistic; 4) mechanistic; 5) post-mechanistic. All perception is channeled through one of two executives, PERCEP (pre- and post-mechanistic) and MCHPRCP (all others). Several flags control what sort of perception-induced alterations are permissible.

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**Reposition** (SDG) The final stage in *Structure Diagram Generation*, in which molecules are translated (shifted) to maximize the distance between them while maintaining their size as much as possible. Consists of two steps:

- a) Analytic placement.
- b) Dynamic repositioning. The *fragments* are treated as if they were charged particles that repel one another. They are allowed to move under each other's forces until they come to rest at equilibrium.

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**Stereochemistry** Most important stereochemistry of organic molecules can be represented in CAMEO, i.e. enantiomers and double bond stereoisomers. The notable omission is allene stereochemistry. A racemic mixture is represented by the absence of wedged or dotted bonds. Mixtures of *cis/trans* isomers are represented by labeling the double bond with a "U"; see Appendix B for a discussion. On rare occasions, usually in bridged ring systems, the program is unable to design a diagram in which a double bond has the correct *cis* or *trans* substituent pattern; an "I" is drawn beside such bonds to indicate that their stereochemistry is opposite that shown.

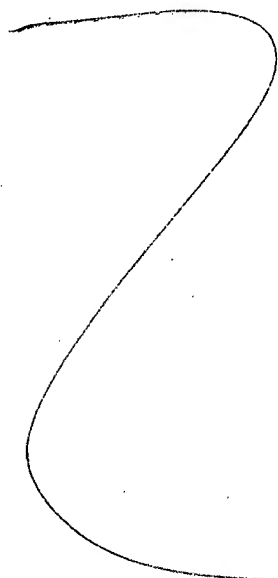
**Structure** One or more molecules that collectively constitute a chemical system undergoing reaction or emerging from reaction. The structure is a unit of storage; it is described by an A/B table, a tree node number, and more or less information about its role as a starting material and/or product.

**Structure Diagram Generation (SDG)** The introduction or optimization of the two-dimensional coordinates in a connection table, especially for the purpose of realizing an aesthetic drawing. Consists of: a) Regularizing bond lengths and angles, and rendering rings in a conventional orientation. b) Redistributing molecules within the plotting area. Cf. *Reposition*.

**Symmetry** An object is symmetric if it contains components that are equivalent by some specified criteria. Equivalent components belong to the same "equivalence class," or "orbit." Frequently there are several orbits in one molecule, e.g. the two in butane.

Of the several types of chemical symmetry known, the one that reflects equivalent chemical reactivity is configurational symmetry.

**Symmetry-Reduced A/B (SRAB)** (Symmetry) The smallest subset of the A/B sufficient to reproduce the chemistry of the parent. In cyclohexane, for example, any one atom (bond) is representative of the entire molecule. Limiting attention to the SRAB saves computation time and avoids duplicate products due to symmetry. Reactions which involve more than one atom (bond), however, such as periodate oxidation of vicinal diols, may not rely upon the SRAB.



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As has been seen, some approaches to isomorphism also yield symmetry, and vice versa. There is a fundamental reason why the two problems are related: a simple proof shows that they are formally equivalent; any method to solve one can be modified to solve the other.<sup>4</sup> On a practical level they appear similar because some solutions to both involve partitioning or growing paths, resulting in overlap of these algorithms.

#### Placement in CAMEO

Before describing implementation details, it is shown how SP and ISI are situated within CAMEO. Fig. 4.4 highlights the overall program flow. Symmetry perception occurs during the middle of perception (whether graphic, mechanistic, pre- or post-mechanistic). CCT-coding occurs only at the end of pre- and post-mechanistic perception, i.e. once for the starting material and once for each product. Reaction intermediates may be perceived during the mechanistic phase but are not ordinarily CCT-coded. Because of this arrangement SP is needed and executed much more often than CCT-coding. It therefore made sense to develop an SP procedure that was fast on its own without concern for obtaining a CCT.

The symmetry algorithm requires stereochemical perception information, and must therefore reside after the point in the perception sequence where that is derived. CCT-coding could be performed at any time afterwards, and is performed at the end of a perception pass. Record is kept of which structures have been coded, so that ISI will merely check which structures are not coded, and codes them.

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#### Implementation of Symmetry Perception in CAMEO

The approach we have taken to symmetry perception is entirely original, as it was conceived and implemented without benefit of the literature. Upon review of the literature it is found to be similar to that published by Shelley and Munk more than a decade earlier,<sup>20,22</sup> and that of Balaban *et al.* several years ago.<sup>8,2,29</sup> The basic strategy is Iterative Vertex Partitioning (IVP), in which local molecular irregularities are propagated through the molecule until all atoms are partitioned into a stable number of distinct types. Because our implementation was conceived independently it is somewhat different. For one thing our symmetry perception has the extra responsibilities described in the previous section. For another, Shelley and Munk's algorithm, despite its suggestions, does not know what to do with stereochemistry or aromaticity, while Balaban *et al.*'s approach cannot treat stereochemistry at all without resorting to path-growing; our method treats these features routinely and rapidly. Finally, our algorithm is the first we know of not based on path growing to yield bond symmetry as well as atom symmetry.

fig. 4.5:

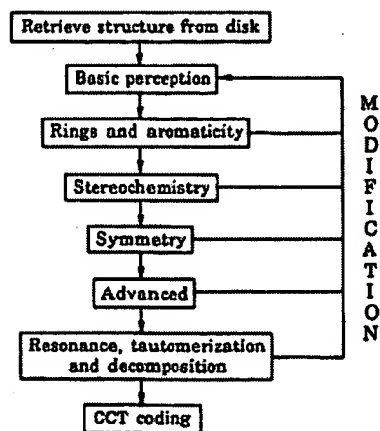


Figure 4.5. The perception phase

Fig. 4.9:

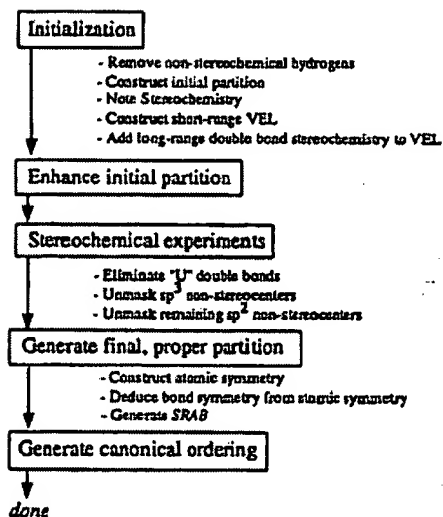


Figure 4.9. Symmetry perception

Table 4.3:



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Table 4.3. Symmetry perception timing information

Structure	No. Equivalence Classes: Atoms/Bonds <sup>a</sup>	Passes: Soft + Hard <sup>b</sup>	CPU <sup>c</sup> (10 <sup>-2</sup> sec)
methane	1 / 0	0 + 0	0.1
ethane	1 / 1	1 + 1	0.3
propane	2 / 1	1 + 1	0.4
butane	2 / 2	1 + 1	0.7
decane	5 / 5	4 + 1	2.4
decanol	11 / 10	4 + 0	1.9
2-cyanonaphthalene	12 / 13	4 + 0	2.3
benzopyrene	5 / 6	3 + 1	8.3
adamantane	2 / 1	1 + 1	2.1
adamantan-1-ol	5 / 4	2 + 1	2.3
adamantan-2-ol	6 / 5	3 + 1	2.8
cubane	1 / 1	1 + 1	2.0
moebius cubane	1 / 1	1 + 1	2.0
moebius cubane <sup>d</sup>	1 / 2	7 + 3	6.1
cubanol	5 / 4	3 + 1	2.1
benzene	1 / 1	1 + 1	1.3
naphthalene	3 / 4	2 + 1	2.2
retinol	20 / 20	6 + 1	9.3
strychnine	25 / 31	3 + 0	6.4
morphine	25 / 29	2 + 0	6.0
muscarine	13 / 13	6 + 1	4.5
isoprene	5 / 4	1 + 0	0.5
2-methyl-2-butene	5 / 4	4 + 1	1.3
cyclohexene	3 / 4	4 + 1	1.7
1-methylcyclohexene	7 / 7	2 + 0	1.2
1,2-dimethyl-cyclohexene	4 / 5	3 + 1	2.3
2,2-dimethylpropane	2 / 1	1 + 1	0.8
glycerol	4 / 3	2 + 1	1.0
penicillanic acid	14 / 15	5 + 1	4.0
inositol	18 / 18	27 + 0	20.1
1-butene	4 / 3	1 + 0	0.4
cis-2-pentene	5 / 4	2 + 0	0.8
U-2-pentene	5 / 4	2 + 0	0.9
22 as drawn	24 / 28	11 + 2	19.1
racemic 22	18 / 19	5 + 1	11.2
3-methyl-tridecane	14 / 13	4 + 0	2.8
2-methyl-tridecane	13 / 12	6 + 1	3.8
7-methyl-tridecane	8 / 7	3 + 1	3.3

<sup>a</sup>Note that the numbers increase with decreasing symmetry. An asymmetric molecule has an equivalence class for every one of its atoms and bonds.

<sup>b</sup>Structures for which the number of hard passes is zero necessarily lack any (configurational) symmetry.

<sup>c</sup>By comparison, it took 499 sec to find the 9592 primes between 2 and 100,000, inclusive, factoring every odd number.

<sup>d</sup>With ring membership checks.

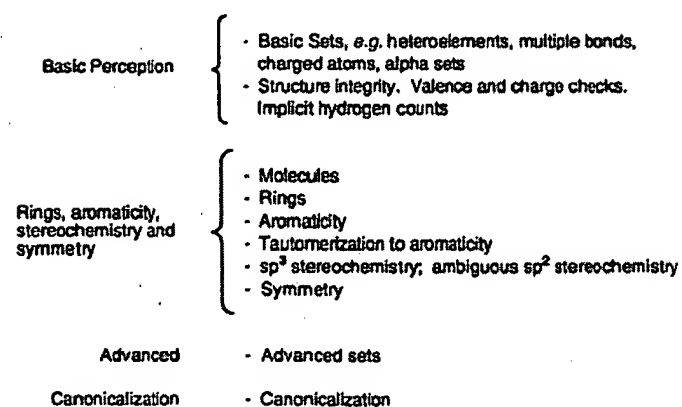


Figure 5.4. Components of the perception phase

**Claim Rejections - 35 USC 103**

7. The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

**8. Claims 1, 5, 9 are rejected under 35 U.S.C. 103(a) as being unpatentable over (Hu et al. or Shelley et al. or Fan) in view of Helson (thesis).**

9. Hu et al. disclose computer perception of topological symmetry from a connection table (see abstract).

10. Shelley et al. also disclose computer perception of topological symmetry from a connection table (see pg. 247).

11. Fan et al. disclose detection of constitutionally equivalent atoms from a connection table (see page 654).

12. Hu et al. or Shelley et al. or Fan et al. do not expressly disclose positioning the atoms and bonds.

13. Helson discloses positioning in chapter 3 (cameo) of symmetrical structures (chapter 4).

14. It would have been obvious to one of ordinary skill in the art at the time of the invention to modify each base teaching with the secondary teaching because

Helson discloses displaying positioning the atoms and bonds and its benefits, namely that disclosed in 1-5 of the thesis.

**15. Claims 13-27 are rejected under 35 U.S.C. 103(a) as being unpatentable over (Hu et al. or Shelley et al. or Fan et al.) in view of Helson and in further view of (Chem 3D [of record] and Razinger et al. [of record]).**

16. Hu et al. or Shelley et al. or Fan et al. do not expressly disclose all *examples* of symmetry operations.

17. Chem3D discloses symmetry operations and properties and their manipulation in molecular modeling and analysis (chapters 4-5).

18. It would have been obvious to one of ordinary skill in the art at the time of the invention to modify the base teaching with the secondary teaching because Razinger et al. expressly discloses the importance of studying the various symmetries (first two paragraphs, col. 1, page 197) and carrying out and representing various chemical symmetry operations (chapter 4-5) when modeling and analyzing chemical structures.

#### **Response to Arguments**

19. Applicant's arguments, filed 5/23/2007, have been carefully considered and are not persuasive.

20. Applicants are thanked for discussing the references; such discussion considerably eases the burden on the Examiner. They have been carefully considered.

21. Applicants state:

The Office Action objects to the last filed Information Disclosure Statement (IDS) as being overly lengthy and being filed subsequent to the Notice of Allowance. The IDS was not signed as having been reviewed by the Examiner. Rather, citing MPEP § 2004, the Office Action requests technical assistance in reviewing the references cited on the IDS.

This latest IDS, coupled with the IDSs of record include multiple thousands of pages of extremely dense and advanced chemistry.

22. Applicants argue:

MPEP § 609 states "An information disclosure statement filed in accordance with the provisions of 37 C.F.R. 1.97 and 37 C.F.R. 1.98 will be considered by the examiner assigned to the application" (emphasis added). The IDS in the present case was filed in accordance with 37 C.F.R. §§ 1.97 and 1.98. MPEP § 609 continues, "Once the minimum requirements of 37 C.F.R. 1.97 and 37 C.F.R. 1.98 are met, the examiner has an obligation to consider the information." There is no limitation in 37 C.F.R. 1.97 or 37 C.F.R. 1.98 regarding the length or number of the references. Moreover, such requirements are not provided in MPEP § 609.04(a), which provides

23. In fact, the office may require Applicants to explain the details of improvement over the art of record (MPEP 704.14(a)). See form paragraphs

7.121, 7.110:

¶ *7.121 Details of Improvement Over the Prior Art*

In response to this requirement, please state the specific improvements of the subject matter in claims [1] over the disclosed prior art and indicate the specific elements in the claimed subject matter that provide those improvements. For those claims expressed as means or steps plus function, please provide the specific page and line numbers within the disclosure which describe the claimed structure and acts.

¶ *7.110 Art Suggested as Relevant*

The information is required to enter in the record the art suggested by the applicant as relevant to this examination in [1].

24. However, in view of Applicant's response to the Examiner's request for assistance, such requirement is not necessary at this time and the Examiner provides full faith and credit that Applicants have fulfilled their duty to disclose under 37 CFR 1.56 (MPEP 2001).

25. Applicants argue:

**Rejection of Claims Under 35 U.S.C. 101**

Claims 1, 5, 9, and 13-27 are rejected under 35 U.S.C. 101 as allegedly being directed to non-statutory subject matter. The Office Action asserts that the claims do not produce a concrete useful and tangible result. Applicant disagrees with the assertion that the claims are directed to non-statutory subject matter. Moreover, this rejection follows a Notice of Allowance for the same claims. Such piecemeal prosecution is generally disfavored. Nevertheless, solely in an effort to expedite allowance, independent claims 1, 5, and 9 have been amended to include "outputting a representation of a chemical structure." Applicant respectfully requests the rejection be removed in view of the amendment.

26. The 101 rejections are withdrawn. Claim 1 is drawn to a practical application. Amended claim 5 is statutory because the code blocks are claimed in conjunction with hardware, thus the claim is not drawn to software per se. Claim 9 is statutory because it is directed to a computer-program product and thus is not drawn to software per se (MPEP 2106.01 (I)):

Since a computer program is merely a set of instructions capable of being executed by a computer, the computer program itself is not a process and USPTO personnel should treat a claim for a computer program, without the computer-readable medium needed to realize the computer program's functionality, as nonstatutory functional descriptive material. When a computer program is claimed in a process where the computer is executing the computer program's instructions, USPTO personnel should treat the claim as a process claim. See paragraph IV.B.2(b), below. When a computer program is recited in conjunction with a physical structure, such as a computer memory, USPTO personnel should treat the claim as a product claim. See paragraph IV.B.2(a), below.

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27. Applicant's arguments with respect to the art are not persuasive.

28. Applicants argue:

discussion is limited to the *perception* of symmetry, not positioning symmetrically equivalent atoms and bonds in a chemical structure. For example, at page 246, the Helson thesis states "Symmetry perception occurs during the middle of perception...." The next paragraph continues, "The symmetry algorithm requires stereochemical perception information, and must therefore reside after the point in the perception sequence where that is derived." There is no discussion of positioning atoms – whether they are symmetrically equivalent or not – at page 246 of the Helson thesis. Likewise, Figure 4.5, which is referenced at page 246, "reveals the Perception Phase in greater detail" (p. 246), by showing the steps covered in the perception phase of the CAMEO program, including evaluating rings and aromaticity, stereochemistry and symmetry, as well as other factors. Again, there is no teaching or suggestion to position symmetrically equivalent atoms in any way, let alone "in accordance with the identified symmetry," as required by the claims.

29. Pages 4-5 (intro in thesis) disclose:

CAMEO's program flow can be broadly divided into three activities: **graphics, perception and analysis.** In the **graphics** phase materials and conditions are entered and products are displayed. During **perception** important molecular features such as rings, functionality and symmetry are noted for use in the analysis phase. Analysis is conducted by one of

This dissertation is concerned with four projects undertaken within the CAMEO program:

- 1) Simulation of carbene chemistry.
- 2) Perception of configurational symmetry of organic molecules.
- 3) Derivation of a canonical ordering and representation of a chemical structure, referred to as canonicalization.
- 4) Structure diagram generation, i.e., the construction of conventional two-dimensional representations of organic molecules from their connection tables.



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Implementation in CAMEO

In CAMEO, SDG is divided into two independent processes: SDG proper, referred to as "redrawing," and positioning of the resulting molecules, called "repositioning." Both facilities exist as independent packages of routines that may be called to serve different occasions; they are not rigidly tied to any particular phase of the program. In fact, repositioning does not even require perception, although redrawing does. The two executive

30. The claims require:

identifying from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure;

- 1) wherein the instance of symmetry includes symmetrically equivalent atoms and bonds;

See, for example:

**CHAPTER 4. DETECTION OF SYMMETRY AND  
DUPLICATE PRODUCTS**

This chapter examines why symmetry perception (SP) and identical structure identification (ISI) are important, the possible ways to achieve them, and how they have been implemented in the CAMEO program.

- 8) Symmetry. Perhaps the hardest aesthetic attribute to detect algorithmically is balance: the symmetrical distribution of like groups, and also the even distribution of white space. Consider o-diethylbenzene (Fig. 3.40). In drawing A the alkyl chains are unsymmetrical (i.e. there is no C<sub>2</sub> axis, loosely speaking), while both drawings B and C

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are symmetrical, and look better for it. Similarly, tributyl tin hydride looks better when its chains are symmetrically directed (Fig. 3.41, B) than otherwise (A).

The obvious way to assess graphical symmetry would be to check if topologically equivalent atoms occupied "graphically equivalent" positions, whatever that would mean. Although this route would be

a-positioner positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry; and

- 2)

31. The inventor's thesis discloses, at least:

**Algorithm 3.6. Dynamic repositioning engine**

- 1) Initialize
- 2) Calculate forces and tensions
  - a) Assess interactions between boxes
  - b) Assess interactions between boxes and walls
  - c) Sum forces. The following variables are calculated:
    - i. NetFMag(): Magnitude of net force for every box
    - ii. SumNetFMag: Sum the NetFMag's
    - iii. Minimum, maximum and sum of all boxes' tensions
- 3) Accept or Reject
  - a) Accept or Reject the last movement
  - b) Modify Response (attenuation) accordingly
  - c) Evaluate Still\_Strained and Still\_Tensed flags
  - d) If Reject: restore previous coordinates; reduce shift vectors by the same amount that Response was just decreased
  - e) If Accept:
    - i. If so directed, scale every box's net force vector in proportion to the tension acting on it
    - ii. Locate nearest blocking object, and reduce shift if necessary
    - iii. Calculate shift vectors and apply to boxes
    - iv. Clear Still\_Moving if no box has moved a significant amount
- 4) Resume at step 2 unless the maximum number of passes is exceeded or Still\_Moving is clear
- 5) Post-processing
  - a) Calculate "badness" of system: the average tension per box.
  - b) Determine if any box is inhibited

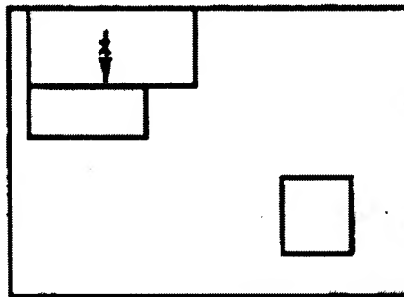


Figure 3.34. Dynamic repositioning stymied by jamming. The top box is blocked by the lower, and so neither moves.



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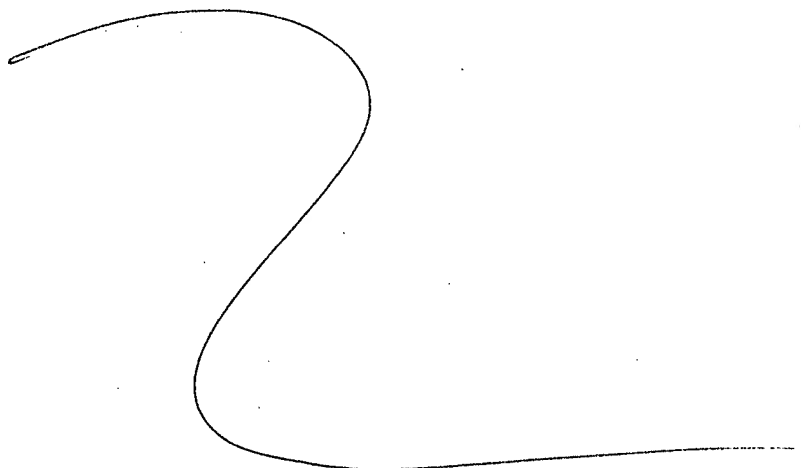
## 32. Applicants argue:

*Hu et al., Shelley et al., or Fan in view of the Helson thesis*

Claims 1, 5, and 9 are rejected under 35 U.S.C. 103(a) as being anticipated by *Hu et al.*, *Shelley et al.*, or *Fan* in view of the Helson thesis. Applicant respectfully disagrees. To establish a prima facie case of obviousness, all claim limitations must be taught or suggested by the prior art. MPEP § 2143.03. As discussed above, the Helson thesis does not teach or suggest "positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in

accordance with the identified symmetry," as required by independent claims 1, 5, and 9. The combination of Helson with Hu *et al.*, Shelley *et al.* or Fan does not cure this deficiency. As explained in more detail in the Response to Office Action dated May 24, 2006, the Hu abstract is concerned with the detection of topological symmetry, in a chemical structure, not the expression of such symmetry in a chemical structural diagram. Shelley, like Hu, teaches an algorithm for detecting topological symmetry. Similarly, Fan, like Hu and Shelley, is concerned with the detection of equivalent atoms. Page 654, abstract ("A simple and efficient algorithm for the perception of constitutionally equivalent atoms in a target molecule is reported.") (emphasis added). None of these references teaches or suggests positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry. Thus, none of the cited references teach all the elements of the claimed invention, either alone or in combination. Accordingly, Applicant submits that the claimed invention is nonobvious in view of Hu or Shelley, or Fan, further in view of the Helson thesis.

33. This is a piecemeal argument. In response to applicant's arguments against the references individually, one cannot show nonobviousness by attacking references individually where the rejections are based on combinations of references. See *In re Keller*, 642 F.2d 413, 208 USPQ 871 (CCPA 1981); *In re Merck & Co.*, 800 F.2d 1091, 231 USPQ 375 (Fed. Cir. 1986). Applicant's basic argument appears to be directed at the Helson thesis. See response presented earlier.



34. Applicants argue:

*Hu et al., Shelley et al., or Fan in view of the Helson thesis, further in view of Chem 3D and Razinger et al.*

Claims 13-27 are rejected under 35 U.S.C. § 103(a) as being obvious in view of Hu, Shelley, or Fan, in view of the Helson thesis, and further in view of Chem 3D and Razinger. Applicant respectfully disagrees. Claims 13-27 depend from claim 1. As explained above, Hu, Shelley, or Fan in combination with the Helson thesis do not teach or suggest positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry. Razinger and Chem3D do not cure this deficiency. As described in more detail in the Response to Office Action dated May 24, 2006, Razinger, like Hu, Shelley and Fan merely discloses algorithms for the detection of symmetry. Razinger provides no further accordance with the identified symmetry," as required by independent claims 1, 5, and 9. The combination of Helson with Hu *et al.*, Shelley *et al.* or Fan does not cure this deficiency. As explained in more detail in the Response to Office Action dated May 24, 2006, the Hu abstract is concerned with the detection of topological symmetry, in a chemical structure, not the expression of such symmetry in a chemical structural diagram. Shelley, like Hu, teaches an algorithm for detecting topological symmetry. Similarly, Fan, like Hu and Shelley, is concerned with the detection of equivalent atoms. Page 654, abstract ("A simple and efficient algorithm for the perception of constitutionally equivalent atoms in a target molecule is reported.") (emphasis added). None of these references teaches or suggests positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry.

35. This is a piecemeal argument. In response to applicant's arguments against the references individually, one cannot show nonobviousness by attacking references individually where the rejections are based on combinations of references. See *In re Keller*, 642 F.2d 413, 208 USPQ 871 (CCPA 1981); *In re Merck & Co.*, 800 F.2d 1091, 231 USPQ 375 (Fed. Cir. 1986). Applicant's argument appears to be directed at the Helson thesis. See response presented earlier.

**Conclusion**

**36. THIS ACTION IS MADE FINAL.** Applicant is reminded of the extension of time policy as set forth in 37 CFR 1.136(a).

37. A shortened statutory period for reply to this final action is set to expire **THREE MONTHS** from the mailing date of this action. In the event a first reply is filed within **TWO MONTHS** of the mailing date of this final action and the advisory action is not mailed until after the end of the **THREE-MONTH** shortened statutory period, then the shortened statutory period will expire on the date the advisory action is mailed, and any extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of the advisory action. In no event, however, will the statutory period for reply expire later than **SIX MONTHS** from the mailing date of this final action.

**38. Any inquiry concerning this communication or earlier communications from the examiner should be:**

directed to: Dr. Hugh Jones telephone number (571) 272-3781,  
Monday-Thursday 0830 to 0700 ET,

**or**

the examiner's supervisor, Kamini Shah, telephone number (571) 272-2279.

Any inquiry of a general nature or relating to the status of this application should be directed to the Group receptionist, telephone number (703) 305-3900.

**mailed to:**

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Washington, D.C. 20231

**or faxed to:**


(703) 308-9051 (for formal communications intended for entry)

**or** (703) 308-1396 (for informal or draft communications, please label  
*PROPOSED* or *DRAFT*).

Dr. Hugh Jones

Primary Patent Examiner

August 5, 2007

  
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PRIMARY PATENT EXAMINER  
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